

Pure decoherence in quantum systems

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Abstract

A popular model of decoherence based on the linear coupling to harmonic oscillator heat baths is analyzed and shown to be inappropriate in the regime where decoherence dominates over energy dissipation, called pure decoherence regime. The similar mechanism essentially related to the energy conservation implies that, on the contrary to the recent conjectures, chaotic environments can be less efficient decoherers than regular ones. Finally, the elastic scattering mechanism is advocated as the simplest source of pure decoherence.

Decoherence became one of the most popular topics in the physical literature of the last decade [1-4]. This is mainly due to the progress in experimental techniques allowing to observe the onset of decoherence at the most interesting regime i.e. at the border between quantum and classical worlds [5]. Another motivation is a destructive role of decoherence in the possible future technology based on quantum information processing [6]. Despite the fact that the theoretical models of decoherence exist at least for 40 years [7] a closer look at certain aspects of these theories reveals inconsistencies and interpretational problems. We shall use the following definition: *Decoherence is an irreversible, uncontrollable and persistent formation of quantum correlations (entanglement) of the system with its environment.*

Usually, decoherence is accompanied by *dissipation* i.e. the net exchange of energy with environment. For the sake of clarity we shall restrict ourselves to the case of *pure decoherence* called also *dephasing* for which the process of energy dissipation is negligible. This situation occurs in two cases: A) for system's Hamiltonian H_S commuting (approximatively) with the system-bath interaction Hamiltonian H_{int} ; B) for the initial states of S which evolve very slowly under the dynamics governed by H_S on the time scale of decoherence processes. In both cases we can disregard the presence of system's Hamiltonian H_S in the derivations concerning decoherence processes. As an example of B) we can consider a system equivalent to a 1-dimensional particle in a symmetric double-well potential coupled to a bath. In the semiclassical regime we can restrict ourselves to the 2-dimensional Hilbert space of initial states spanned by the lowest lying almost degenerated Hamiltonian eigenstates [8]. The second example is a heavy particle interacting with a medium. As initial states for its center of motion we can choose superpositions of well-localized wave packets with small enough kinetic energies. For decoherence effects grow with the size of the particle while the kinetic energy exchange decreases we are again in the pure decoherence regime.

Pure decoherence is supposed to be the main ingredient of the theory explaining the apparent absence of superpositions of macroscopically distinguishable states and the transition from quantum to classical world. Indeed, the explanation of the rapid decay of quantum correlations between "Schrödinger cat" states should not essentially depend on the energy difference between $|dead\ cat\rangle$ and $|alive\ cat\rangle$ but is rather related to the distinguishability of these states described in terms of certain collective observables which are coupled to the environment.

In this letter we show that the most popular model of quantum open system based on

the linear coupling to the harmonic oscillator bath is inadequate in the pure decoherence regime. Using a unifying approach in terms of reservoir's spectral function we also show that, contrary to the recent conjecture, chaotic environments can be less efficient decoherers than regular ones at least for pure decoherence case.

The first problem can be understood in simple physical terms. Namely, pure decoherence in the open system must be accompanied by the irreversible perturbation of the environment's state but the energy of the environment should be asymptotically preserved. However, the linear coupling to the bosonic environment implies that the only change of its state is caused by irreversible processes of emission and absorption of single bosons which must alter the environment's energy. The energy exchange can be reduced by a strong coupling to low energy bosons what in turn produces infrared divergencies. Those divergencies change completely the physical interpretation of the model, in particular the decomposition of the total system into the open system S and the reservoir R , what seems not to be taken into account in the literature [9,10].

Spin-boson model [11]. To explain this effect in a rigorous way we consider a two level system coupled linearly to the bosonic reservoir that is defined in terms of fields satisfying canonical commutation relations $[a(\omega), a^\dagger(\omega')] = \delta(\omega - \omega')$, a single-boson Hilbert space $L^2[0, \infty)$, a single-boson Hamiltonian h_1 , $(h_1 f)(\omega) = \omega f(\omega)$ and the second quantization Hamiltonian

$$H_B = \int_0^\infty d\omega \omega a^\dagger(\omega) a(\omega) \quad (1)$$

acting on the bosonic Fock space $\mathcal{F}_B(L^2[0, \infty))$ with the vacuum state Ω . The general spin-boson Hamiltonian depending on the function ("formfactor") $g(\omega)$ can be written as (σ_k - Pauli matrices)

$$\mathbf{H}_g = H_S + H_B + H_{int}(g) , \quad H_S = \frac{1}{2} \epsilon \sigma_1 \quad (2)$$

where the interaction Hamiltonian is linear in bosonic field and reads

$$H_{int}(g) = \sigma_3 \otimes \int_0^\infty d\omega \omega (\bar{g}(\omega) a(\omega) + g(\omega) a^\dagger(\omega)) . \quad (3)$$

The Hamiltonians act on the Hilbert space $\mathcal{H}_{SB} = \mathbf{C}^2 \otimes \mathcal{F}_B(L^2[0, \infty))$. The system Hamiltonian H_S describes the coherent tunneling between two eigenstates of the "position" operator $\sigma_3 \psi_\pm = \pm \psi_\pm$. We assume that this process is much slower then the decoherence i.e. $\hbar/\epsilon \gg \tau_{dec}$. This is precisely the condition for pure decoherence regime in our model which allows to put $\epsilon = 0$ in (3) and leads to

$$\mathbf{H}_g = \begin{pmatrix} H_{+g} & 0 \\ 0 & H_{-g} \end{pmatrix} \equiv \text{diag}[H_{+g}, H_{-g}] \quad (4)$$

where

$$H_{\pm g} = \int_0^\infty d\omega \omega a^\dagger(\omega) a(\omega) \pm \int_0^\infty d\omega \omega (\bar{g}(\omega) a(\omega) + g(\omega) a^\dagger(\omega)) \quad (5)$$

are van Hove Hamiltonians for the bosonic field which are well-known exactly solvable toy models of renormalization, both in the infrared and ultraviolet regimes. As pure decoherence is a low energy phenomenon we introduce an ultraviolet cut-off ($g(\omega) = 0$ for $\omega > \omega_c$) and for simplicity we assume a power-like low energy scaling

$$|g(\omega)|^2 \sim \omega^{\kappa-1}, \text{ for } \omega \ll \omega_c. \quad (6)$$

The most frequently used in the context of decoherence is the *ohmic coupling* i.e. $\kappa = 0$. Under the assumptions of above one obtains the following rigorous results concerning the existence and properties of the van Hove Hamiltonians [12]:

- 1) $\kappa > 0$, regular case, ground states for $H_{\pm g}$ exist,
- 2) $-1 < \kappa \leq 0$, infrared problem, (includes ohmic case!), $H_{\pm g}$ - bounded from below but ground states do not exist (in the Fock space),
- 3) $\kappa \leq -1$, unphysical case, $H_{\pm g}$ - unbounded from below or do not exist as self-adjoint operators on the Fock space.

The main tool used in the analysis of the Hamiltonian is its diagonalization in terms of unitary Weyl operators $W(f) = \exp\{a(f) - a^\dagger(f)\}$ with $\|f\|^2 = \int_0^\infty |f(\omega)|^2 d\omega < \infty$, acting on the Fock space and satisfying Weyl commutation relations: $W(f)^\dagger = W(-f)$, $W(f)W(h) = e^{-i\text{Im}\langle f, h \rangle} W(f+h)$, $W(f)a(\omega)W(f)^\dagger = a(\omega) + f(\omega)\mathbf{1}$. The vectors $W(f)\Omega$ are called *coherent states* and they form an overcomplete set in the following sense. If for a given vector Ψ from the bosonic Fock space and any $f \in L^2[0, \infty) < \Psi, W(f)\Omega > = 0$, then $\Psi = 0$. Taking into account Weyl relations and $\langle \Omega, W(f)\Omega \rangle = \exp\{-(1/2)\|f\|^2\}$ we obtain

$$|\langle W(f)\Omega, W(h)\Omega \rangle|^2 = e^{-\|f-h\|^2} \leq e^{-(\|f\|-\|h\|)^2}, \quad (7)$$

so $W(f)$ is not unitary on the Fock space unless $\|f\| < \infty$. Introducing now for a given form-factor $g(\omega)$, $\|g\| < \infty$ the unitary operator on \mathcal{H}_{SB} defined as $\mathbf{W}(g) = \text{diag}[W(g), W(-g)]$ we obtain the diagonalized form

$$\mathbf{W}(g)\mathbf{H}_g\mathbf{W}(g)^\dagger = \int_0^\infty d\omega \omega a^\dagger(\omega) a(\omega) - E_g \quad (8)$$

where $E_g = \langle g, h_1 g \rangle = \int_0^\infty \omega |g(\omega)|^2 d\omega$. Therefore, the degenerated ground states of \mathbf{H}_g are given by

$$\mathbf{H}_g \Phi_\pm(g) = -E_g \Phi_\pm(g), \quad \Phi_\pm(g) = \psi_\pm \otimes W(\pm g)\Omega. \quad (9)$$

Obviously, in our setting the regular case 1) ($\kappa > 0$) corresponds to the condition $\|g\| < \infty$. Two degenerated ground states of the Hamiltonian \mathbf{H}_g should be interpreted as the states of a *dressed spin* which consists of a *bare spin* and a *cloud* of virtual bosons represented by the coherent states $W(\pm g)\Omega$. The dressed system is decoupled from the environment and its dynamics is trivial.

The case 2) ($-1 < \kappa \leq 0$) corresponds to $\|g\| = \infty, E_g < \infty$. In principle, the states $\Phi_\pm(g)$ treated as limits of "normal" states from the Hilbert space \mathcal{H}_{SB} with $\|g\| \rightarrow \infty$ can exist in the sense of state functionals on the algebra of observables. But in this case they are *disjoint*, i.e. they define nonequivalent representations of the algebra of observables (van Hove phenomenon [12]). Formally, it follows from the formula $\Phi_+(g) = \sigma_1 \otimes W(2g)\Phi_-(g)$ which for $\|g\| \rightarrow \infty$ indicates that there exists no unitary operator which transforms $\Phi_-(g)$ into $\Phi_+(g)$ [13]. Physically, it means that their superpositions are indistinguishable from their mixtures (*superselection rule*). Some authors invoke this mechanism to describe the emergence of classical observables for quantum systems [14,16]. This phenomenon should be called *static decoherence* because the disjointness is a permanent feature of these states. Although from the mathematical point of view this is an attractive approach, on the other hand it can lead to profound interpretational difficulties, e.g. unphysical superselection rules in quantum electrodynamics [16,17].

We invoke now the standard dynamical approach to decoherence in open systems applied to our spin-boson model. As an initial state of the total system one chooses the product state

$$\Psi_{in} = \psi \otimes \Omega, \quad \psi = \alpha_- \psi_- + \alpha_+ \psi_+, \quad \alpha_\pm \in \mathbb{C} \quad (10)$$

satisfying

$$|\langle \Psi_{in} | \Phi_\pm(g) \rangle|^2 = e^{-\|g\|^2}, \quad E(\Psi_{in}) = \langle \Psi_{in} | \mathbf{H}_g | \Psi_{in} \rangle = 0, \quad (11)$$

computes its time evolution governed by the Hamiltonian (4)(5)

$$\Psi(t) = e^{-it\mathbf{H}_g} \Psi_{in} = \exp\{i(tE_g - \text{Im} \langle g | g_t \rangle)\} (\alpha_- \psi_- \otimes W(g_t - g)\Omega + \alpha_+ \psi_+ \otimes W(g - g_t)\Omega) \quad (12)$$

where $g_t(\omega) = e^{-i\omega t}g(\omega)$ and calculates the reduced density matrix for spin

$$\rho_t = \text{Tr}_B |\Psi(t)\rangle \langle \Psi(t)| = \begin{pmatrix} |\alpha_+|^2 & \alpha_+ \bar{\alpha}_- e^{-\gamma t} \\ \bar{\alpha}_+ \alpha_- e^{-\gamma t} & |\alpha_-|^2 \end{pmatrix} \quad (13)$$

with

$$\gamma_t = 2\|g - g_t\|^2 \leq 8\|g\|^2. \quad (14)$$

Usually, one discusses the structure of the reduced density matrix (13) only, and identifies γ_t with the decoherence factor. It follows from (14) that decoherence is complete only if $\|g\| = \infty$ i.e. for a singular coupling. To obtain an asymptotically exponential decay of the off-diagonal elements of the reduced density matrix (13) we must assume

$$0 < \gamma = \lim_{t \rightarrow \infty} \frac{\gamma_t}{t} = \lim_{t \rightarrow \infty} \int_0^{\omega_c} \omega^2 |g(\omega)|^2 \frac{1 - \cos \omega t}{t \omega^2} d\omega = \pi \lim_{\omega \rightarrow 0} \omega^2 |g(\omega)|^2. \quad (15)$$

This result agrees with the standard wisdom relating the pure decoherence rate to the value at $\omega = 0$ of the *spectral density function* [4,18]

$$\hat{R}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} \langle R(t) R \rangle_B dt \quad (16)$$

where R is a bath's operator appearing in the interaction Hamiltonian $\sigma_3 \otimes R$ and $\langle \cdot \rangle_B$ is an average with respect to the environment's state. It is a special case of the quantum *fluctuation - dissipation theorem* which in fact should be called in this context a "fluctuation-decoherence theorem". For our model $R = \int d\omega \omega (\bar{g}(\omega) a(\omega) + h.c.)$ and hence $\hat{R}_0(\omega) = 2\pi\omega^2 |g(\omega)|^2$ where the subscript "0" indicates the zero-temperature (vacuum) state of the bath. However, a non zero value of γ means $\kappa = -1$ which is the unphysical (subohmic) case 2). The situation is slightly less singular for the temperature $T > 0$. It is easy to check that for $\omega \ll T$ (we put $\hbar \equiv k_B \equiv 1$) $\hat{R}_T(\omega) \simeq (T/\omega) \hat{R}_0(\omega)$ and hence the condition of finite decoherence rate is satisfied for the ohmic case $\kappa = 0$. The same ohmic assumption is made in the derivation of the popular Caldeira-Leggett equation for the quantum Brownian particle coupled to harmonic oscillator heat bath[10].

A different physical interpretation of the discussed process follows from the analysis of the state evolution for the total system in the regular case. As for $t \rightarrow \infty$ the traveling wave g_t becomes orthogonal to g the asymptotic form of $\Psi(t)$ possesses the structure of superposition of two triple product states $\psi_{\pm} \otimes W(\pm g)\Omega \otimes W(\mp g_t)\Omega$. Hence, the evolution of the initial product state (10) given by (12) describes the process of formation of the cloud accompanied

by emission of the average energy E_g in a form of coherent traveling waves $\pm g_t$. Therefore, from the physical point of view the discussed model describes a phenomenon which should be called *false decoherence* [19].

Summarizing the above results one can say that the linear coupling to harmonic oscillator bath is not an appropriate model of pure decoherence phenomena. In general, we have two different choices of the formfactor $g(\omega)$ - a singular and a regular one, both leading to difficulties.

The singular coupling (e.g. ohmic, $\kappa = 0$, for $T > 0$ or subohmic, $\kappa = -1$, for $T = 0$), which gives a finite asymptotic decoherence rate in the formal derivation of the reduced density matrix, leads to serious interpretational difficulties due to infrared divergencies. The ground states do not exist in the Fock space, those defined by limiting procedures describe disjoint states for which superposition principle is not applicable. As a consequence the picture of an open system gradually losing its "quantum coherences" is not valid in this case.

For the regular coupling the natural representation of dressed states gives the picture of a "physical dressed system" decoupled from its environment. The choice of the initial product state of a bare system and a bath makes sense only in the unique moment of system's creation followed by the irreversible dressing process. After that, the system cannot be prepared in a such state again. The absence of true decoherence in the regular (superohmic) case is indicated by the relation $\lim_{\omega \rightarrow 0} \hat{R}(\omega) = 0$. It follows that the models based on vacuum fluctuations of the background quantum fields (gravitational, electromagnetic,...) [20] are very unlikely to solve the problem of transition from the quantum to classical world.

Chaotic vs. regular environments. The similar physical mechanism leading to the absence of pure decoherence appears in the case of a bath which is an ensemble of quantum subsystems with chaotic properties. The intuition supported by some heuristic arguments suggests, as it is formulated in [21], that "...one would expect that environments with unstable dynamics will be much more efficient decoherers,...". However, it follows from the previous discussion that the reservoir's energy eigenstates should be degenerated and labeled by other quantum numbers which can be altered without energy modification. On the contrary, for a chaotic system its energy levels are typically nondegenerated due to the mechanism of *level repulsion* [22].

We begin with the physical example as a motivation. Consider a large system (say a

molecule) with a relevant collective, single degree of freedom which can be modeled by a 2-level system as above. This degree of freedom is our open system again, while the internal degrees of freedom of the molecule form a bath which can be treated as a large ensemble of quantum systems.

The simplified mathematical model consists of a 1/2-spin system interacting with an ensemble of N identical M -level quantum systems by means of the following mean-field type Hamiltonian which is an analog of (2)[23]

$$\mathbf{H}_Q = \frac{1}{2}\epsilon\sigma_1 + \sum_{k=1}^N h^{(k)} + \sigma_3 \otimes N^{-1/2} \sum_{k=1}^N Q^{(k)} . \quad (17)$$

Here $h^{(k)}$ is a copy of the Hamiltonian with the spectral resolution $h = \sum_{m=1}^M \epsilon_m |m\rangle\langle m|$, $\epsilon_{m+1} \geq \epsilon_m$ and $Q^{(k)}$ is a copy of an operator $Q = Q^\dagger$, $\text{Tr}Q = 0$. The reference state of environment is assumed to be the product state $\otimes_{k=1}^N \rho^{(k)}$ where $\rho^{(k)}$ is a copy of the microcanonical state giving an uniform probability distribution over all states $|m\rangle$. We assume again, that the tunneling time \hbar/ϵ is much longer than the decoherence time and that the energy ϵ is much smaller than the typical reservoir's constituents energy spacing Δ (compare again [8]). For $N \rightarrow \infty$ the mean-field reservoir's observable $N^{-1/2} \sum_{k=1}^N Q^{(k)}$ behaves like a Gaussian noise and in the Markovian approximation the pure decoherence rate γ for the spin is given by the following version of the fluctuation-dissipation formula

$$\gamma = \frac{1}{2} \lim_{\omega \rightarrow 0} \hat{R}(\omega) , \quad \hat{R}(\omega) = \frac{\pi}{M} \sum_{m,m'=1}^M | \langle m|Q|m' \rangle |^2 \delta((\epsilon_m - \epsilon_{m'}) - \omega) . \quad (18)$$

This formula makes sense also when instead of identical subsystems the reservoir consists of a large random ensemble of quantum systems with Hamiltonians $h^{(k)}$ characterized by the average nearest-neighbour level spacing distribution $p(s)$ with the average Δ . For $\omega \ll \Delta$ only the nearest-neighbour level spacings $s = \epsilon_{m+1} - \epsilon_m$ contribute to the spectral function $\hat{R}(\omega)$ (18) and therefore the difference between the bath consisting of classically integrable or chaotic systems becomes crucial. For the former we expect a Poisson distribution of s while for the later the level repulsion given by $p(s) \sim s^\beta$, $\beta = 1, 2$, or 4 is generically observed [22]. Assuming that the magnitude of the matrix elements $| \langle m+1|Q|m \rangle |$ is not strongly correlated with $\epsilon_{m+1} - \epsilon_m$ we obtain

$$\hat{R}(\omega) \simeq \pi \bar{Q}^2 p(\omega) \quad (19)$$

where \bar{Q}^2 is an averaged value of $|\langle m+1|Q|m\rangle|^2$. As a consequence pure decoherence rate is equal to zero for the chaotic systems while for the regular ones we obtain a finite value of γ .

We have shown that for important models used to analyse environmental decoherence this phenomenon disappears in the limit of pure decoherence. These cases can be easily detected applying the unified approach of spectral density function (16) at $\omega \rightarrow 0$. To avoid the possible influence of approximation procedures we have studied in details an exactly solvable spin-boson model which illustrated both, vanishing pure decoherence and infrared divergencies for the singular choice of the coupling. The proper models of pure decoherence involve *elastic scattering* processes which "for all practical purposes" provide strong enough suppression of quantum superpositions in the macroworld (e.g. Joos and Zeh [7]), [24] or describe quantum Brownian motion [25].

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